Cyclopentane
287-92-3 | DTXSID6024886

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 6.13e-12 cm3/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 8.13e-01

Confidence level: 6.55e-01

Nearest Neighbors from the Training Set

Image not found
Cyclopentane
Measured: 5.16e-12
Predicted: 6.13e-12

Image not found
Cyclohexane
Measured: 7.49e-12
Predicted: 7.04e-12

Image not found
Cyclobutane
Measured: 1.50e-12
Predicted: 1.78e-12

Image not found
Cycloheptane
Measured: 1.25e-11
Predicted: 9.38e-12

Image not found
Dimethylamine
Measured: 6.54e-11
Predicted: 2.85e-11